



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:36 PM UTC

PDB ID : 4EOP / pdb_00004eop
Title : Thr 160 phosphorylated CDK2 Q131E - human cyclin A3 complex with the inhibitor RO3306
Authors : Echalier, A.; Cot, E.; Camasses, A.; Hodimont, E.; Hoh, F.; Sheinerman, F.; Krasinska, L.; Fisher, D.
Deposited on : 2012-04-14
Resolution : 1.99 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

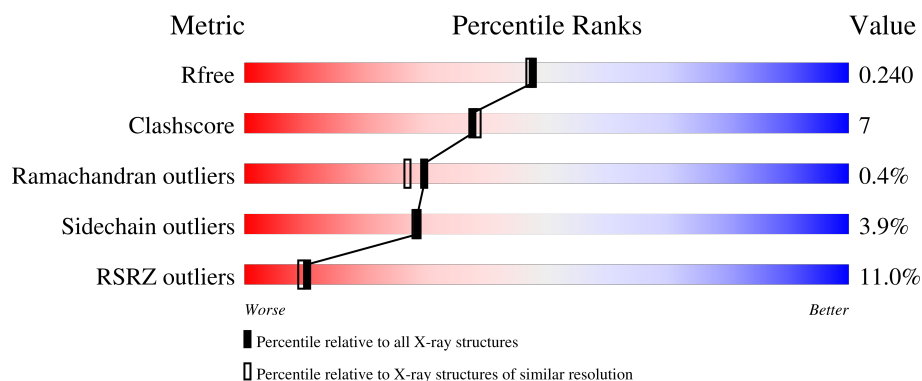
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.99 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	300	6% 83% 14% ...
1	C	300	10% 85% 12% ...
2	B	258	11% 89% 9% .
2	D	258	18% 85% 13% ..

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	1RO	A	301	-	-	X	-
3	1RO	C	301	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9518 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Cyclin-dependent kinase 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	298	Total	C	N	O	P	S	0	4	0
			2420	1568	411	432	1	8			
1	C	297	Total	C	N	O	P	S	0	3	0
			2409	1561	406	433	1	8			

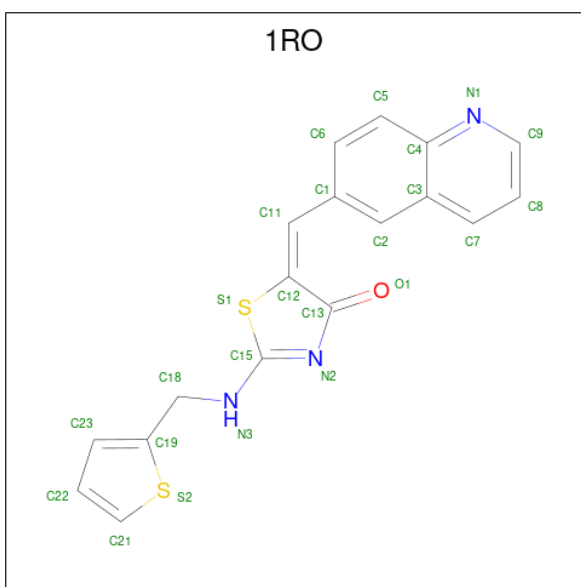
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	PRO	-	expression tag	UNP P24941
A	-1	GLY	-	expression tag	UNP P24941
A	0	SER	-	expression tag	UNP P24941
A	131	GLU	GLN	engineered mutation	UNP P24941
C	-2	PRO	-	expression tag	UNP P24941
C	-1	GLY	-	expression tag	UNP P24941
C	0	SER	-	expression tag	UNP P24941
C	131	GLU	GLN	engineered mutation	UNP P24941

- Molecule 2 is a protein called Cyclin-A2.

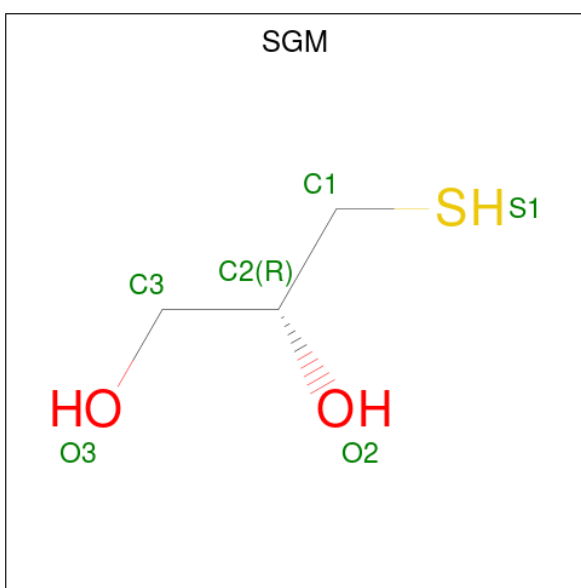
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	257	Total	C	N	O	S	0	2	0
			2094	1356	342	384	12			
2	D	255	Total	C	N	O	S	0	0	0
			2059	1334	335	379	11			

- Molecule 3 is (5E)-5-(quinolin-6-ylmethylidene)-2-[(thiophen-2-ylmethyl)amino]-1,3-thiazol-4(5H)-one (CCD ID: 1RO) (formula: C₁₈H₁₃N₃OS₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			24	18	3	1	2		
3	C	1	Total	C	N	O	S	0	0
			24	18	3	1	2		

- Molecule 4 is MONOTHIOGLYCEROL (CCD ID: SGM) (formula: $C_3H_8O_2S$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	O	S	0	0
			6	3	2	1		

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	1	Total 1	Mg 1	0	0

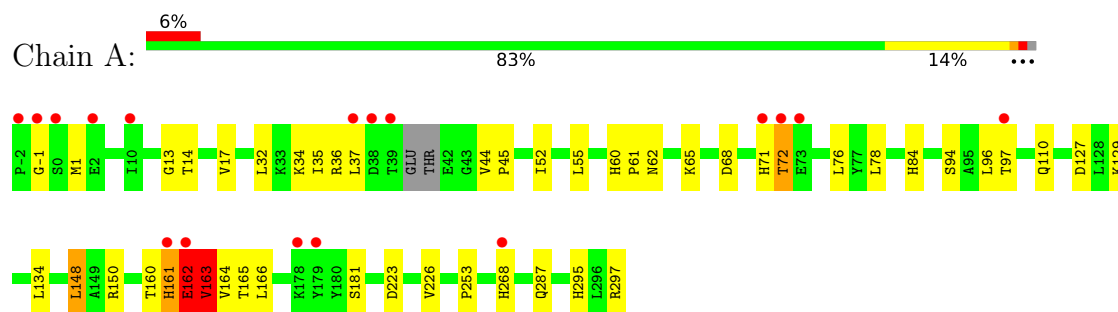
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	170	Total 170	O 170	0	0
6	B	113	Total 113	O 113	0	0
6	C	120	Total 120	O 120	0	0
6	D	78	Total 78	O 78	0	0

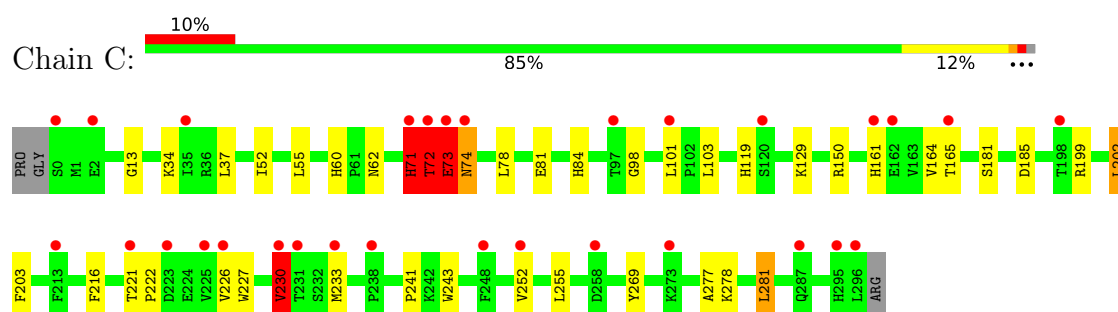
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

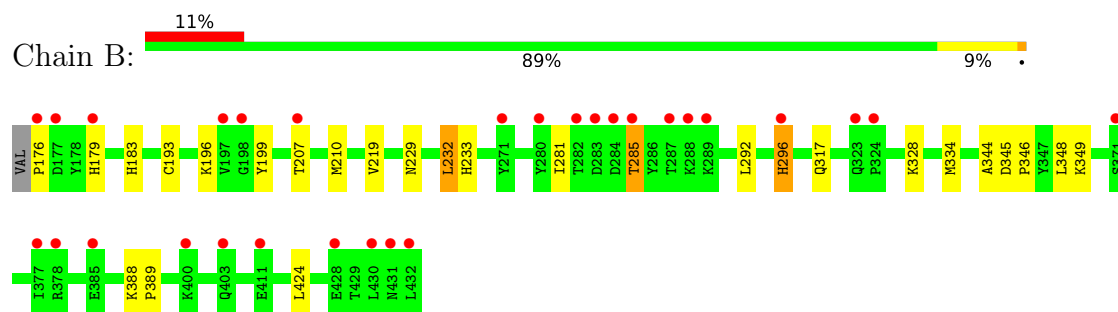
• Molecule 1: Cyclin-dependent kinase 2



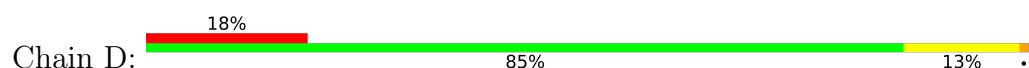
• Molecule 1: Cyclin-dependent kinase 2

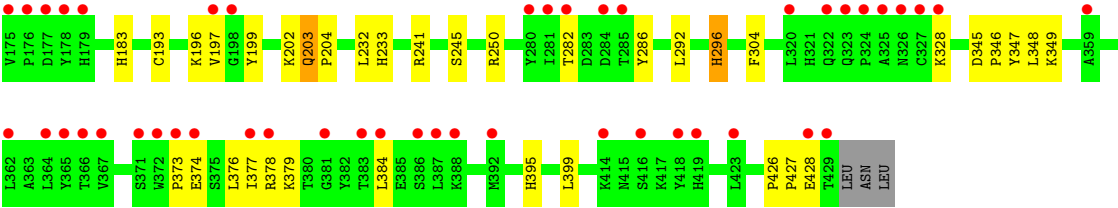


• Molecule 2: Cyclin-A2



• Molecule 2: Cyclin-A2





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	74.78Å 133.39Å 147.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.83 – 1.99 29.83 – 1.99	Depositor EDS
% Data completeness (in resolution range)	98.7 (29.83-1.99) 98.7 (29.83-1.99)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.35 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.216 , 0.241 0.214 , 0.240	Depositor DCC
R_{free} test set	5099 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	29.7	Xtriage
Anisotropy	0.065	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 36.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9518	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.25% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TPO, MG, 1RO, SGM

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.78	2/2470 (0.1%)	0.82	2/3349 (0.1%)
1	C	0.76	6/2459 (0.2%)	0.85	5/3337 (0.1%)
2	B	0.70	0/2145	0.81	0/2911
2	D	0.68	0/2109	0.85	4/2864 (0.1%)
All	All	0.74	8/9183 (0.1%)	0.84	11/12461 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	72	THR	CA-C	-6.39	1.44	1.52
1	C	84	HIS	CG-ND1	-6.16	1.31	1.38
1	A	84	HIS	CD2-NE2	-6.10	1.31	1.37
1	A	84	HIS	CG-ND1	-5.89	1.31	1.38
1	C	71	HIS	CG-ND1	-5.22	1.32	1.38
1	C	71	HIS	CD2-NE2	-5.18	1.32	1.37
1	C	84	HIS	CD2-NE2	-5.07	1.32	1.37
1	C	72	THR	C-O	-5.02	1.18	1.23

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	71	HIS	N-CA-C	7.81	122.20	109.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	73	GLU	N-CA-C	-6.93	103.34	111.03
1	C	74	ASN	N-CA-C	6.89	123.70	114.12
2	D	347	TYR	N-CA-C	5.85	118.60	111.82
1	A	253	PRO	N-CA-C	5.59	117.52	110.70
1	C	71	HIS	CB-CA-C	-5.42	100.91	112.63
1	C	230	VAL	CB-CA-C	-5.42	104.94	112.04
2	D	203	GLN	CA-C-N	5.39	125.21	119.28
2	D	203	GLN	C-N-CA	5.39	125.21	119.28
1	A	166	LEU	N-CA-C	5.28	117.45	111.11
2	D	197	VAL	N-CA-C	5.09	116.42	110.62

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	71	HIS	Peptide
1	C	72	THR	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2420	0	2457	43	0
1	C	2409	0	2441	35	0
2	B	2094	0	2112	20	0
2	D	2059	0	2079	22	0
3	A	24	0	13	9	0
3	C	24	0	13	9	0
4	B	6	0	7	1	0
5	D	1	0	0	0	0
6	A	170	0	0	10	0
6	B	113	0	0	4	0
6	C	120	0	0	5	0
6	D	78	0	0	2	0
All	All	9518	0	9122	128	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 7.

All (128) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:193:CYS:SG	4:B:501:SGM:S1	2.30	1.29
3:A:301:1RO:S1	6:A:482:HOH:O	1.99	1.16
1:C:72:THR:CG2	2:D:296:HIS:NE2	2.11	1.13
1:C:72:THR:HG23	2:D:296:HIS:NE2	1.68	1.08
3:C:301:1RO:S1	6:C:462:HOH:O	2.17	0.99
3:A:301:1RO:O1	3:A:301:1RO:H13	1.62	0.99
3:A:301:1RO:O1	3:A:301:1RO:C2	2.11	0.99
1:C:226:VAL:HB	6:C:459:HOH:O	1.67	0.93
3:C:301:1RO:C2	3:C:301:1RO:O1	2.17	0.93
1:C:72:THR:HG21	2:D:296:HIS:NE2	1.81	0.92
3:C:301:1RO:O1	3:C:301:1RO:H13	1.71	0.88
3:A:301:1RO:C19	3:A:301:1RO:N2	2.43	0.81
1:A:71:HIS:CD2	1:A:72:THR:HB	2.18	0.78
1:A:97:THR:HG22	6:A:441:HOH:O	1.81	0.78
3:C:301:1RO:N2	3:C:301:1RO:C19	2.46	0.75
1:A:60:HIS:HD2	1:A:62:ASN:H	1.34	0.74
1:A:60:HIS:CD2	1:A:62:ASN:H	2.06	0.74
3:A:301:1RO:H13	3:A:301:1RO:C13	2.16	0.74
1:A:52:ILE:HD11	1:A:78:LEU:HD21	1.71	0.72
2:D:282:THR:HG21	2:D:286:TYR:CD2	2.25	0.71
1:C:221:THR:HG21	1:C:241:PRO:O	1.90	0.70
1:C:227:TRP:O	1:C:230:VAL:HG23	1.92	0.69
1:C:129:LYS:HD3	1:C:165[A]:THR:HG21	1.73	0.69
1:C:202:LEU:HD12	1:C:203:PHE:CZ	2.29	0.68
1:C:60:HIS:CD2	1:C:62:ASN:H	2.12	0.68
1:C:252:VAL:HG21	1:C:255:LEU:HD12	1.76	0.67
3:C:301:1RO:H13	3:C:301:1RO:C13	2.25	0.67
3:A:301:1RO:C2	3:A:301:1RO:C13	2.75	0.64
1:A:127:ASP:OD1	1:A:165[A]:THR:HG23	1.97	0.64
1:A:-1:GLY:HA3	1:A:68:ASP:OD2	1.97	0.64
2:B:183:HIS:HB2	2:B:317:GLN:HE22	1.63	0.64
1:A:161:HIS:O	1:A:162:GLU:O	2.17	0.62
1:C:71:HIS:CE1	2:D:304:PHE:HE2	2.17	0.62
1:A:129:LYS:NZ	1:A:165[A]:THR:HG21	2.13	0.62
1:C:13:GLY:HA2	3:C:301:1RO:H2	1.83	0.61
1:C:98:GLY:HA2	1:C:199:ARG:HD3	1.81	0.61
1:C:216:PHE:HB3	1:C:221:THR:HG22	1.82	0.60
1:C:60:HIS:HD2	1:C:62:ASN:H	1.48	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:119:HIS:HD2	6:D:607:HOH:O	1.86	0.58
1:C:227:TRP:O	1:C:230:VAL:CG2	2.50	0.58
2:B:344:ALA:HB1	2:B:348:LEU:HD22	1.85	0.58
1:A:162:GLU:HG2	6:A:408:HOH:O	2.02	0.58
1:C:72:THR:HG1	1:C:73:GLU:C	2.12	0.57
2:B:334[A]:MET:HE3	6:B:619:HOH:O	2.03	0.57
2:B:219:VAL:HG22	2:B:232:LEU:HD11	1.85	0.56
1:A:14[A]:THR:HG21	1:A:148:LEU:HD13	1.88	0.56
1:C:161:HIS:HD2	6:C:439:HOH:O	1.88	0.56
3:C:301:1RO:C2	3:C:301:1RO:C13	2.82	0.55
1:A:94:SER:OG	1:A:295:HIS:HE1	1.89	0.55
1:A:287:GLN:HG2	6:A:515:HOH:O	2.05	0.55
2:B:229:ASN:HD22	2:B:334[B]:MET:HE2	1.71	0.55
1:A:223:ASP:H	1:A:226:VAL:HG12	1.72	0.55
1:A:71:HIS:HB2	1:A:76:LEU:CD1	2.36	0.54
1:C:71:HIS:CE1	2:D:304:PHE:CE2	2.96	0.53
1:A:295:HIS:HD2	1:A:297:ARG:HA	1.74	0.52
1:A:268:HIS:CE1	6:A:485:HOH:O	2.61	0.52
1:A:295:HIS:HD2	1:A:297:ARG:H	1.56	0.52
2:B:233:HIS:HE1	6:B:619:HOH:O	1.93	0.52
2:D:282:THR:HG21	2:D:286:TYR:HD2	1.72	0.52
1:A:295:HIS:CD2	1:A:297:ARG:HA	2.45	0.51
2:B:346:PRO:O	2:B:349:LYS:HG2	2.10	0.51
1:A:181:SER:HB3	6:A:476:HOH:O	2.11	0.51
6:C:420:HOH:O	2:D:296:HIS:HD2	1.93	0.51
2:B:176:PRO:HA	2:B:179[A]:HIS:CG	2.46	0.50
1:A:13:GLY:HA2	3:A:301:1RO:H2	1.94	0.50
1:C:52:ILE:HD11	1:C:78:LEU:HD21	1.94	0.49
1:A:129:LYS:HZ2	1:A:165[A]:THR:HG21	1.78	0.48
1:C:277:ALA:O	1:C:281:LEU:HD22	2.13	0.48
2:D:282:THR:HG22	2:D:282:THR:O	2.13	0.48
2:D:374:GLU:HA	2:D:377:ILE:HD12	1.95	0.48
2:D:346:PRO:O	2:D:349:LYS:HG2	2.13	0.48
1:A:295:HIS:HD2	1:A:297:ARG:N	2.12	0.47
1:C:227:TRP:CE2	1:C:233:MET:HE1	2.50	0.47
1:C:73:GLU:HB3	1:C:74:ASN:ND2	2.30	0.46
1:C:81:GLU:O	3:C:301:1RO:H9	2.15	0.46
1:C:119:HIS:HE1	1:C:185:ASP:OD2	1.98	0.46
2:B:207:THR:HG23	2:B:210:MET:H	1.78	0.46
1:C:227:TRP:CZ2	1:C:233:MET:HE1	2.51	0.46
1:A:161:HIS:O	1:A:162:GLU:C	2.58	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:HIS:CG	1:A:61:PRO:HD2	2.51	0.45
1:A:297:ARG:HD2	6:A:487:HOH:O	2.16	0.45
1:A:129:LYS:HZ3	1:A:165[A]:THR:HG21	1.80	0.45
1:A:94:SER:OG	1:A:295:HIS:CE1	2.70	0.45
1:C:202:LEU:HD12	1:C:203:PHE:CE2	2.52	0.45
3:A:301:1RO:N2	3:A:301:1RO:C23	2.79	0.44
2:B:285:THR:HG22	6:B:699:HOH:O	2.15	0.44
2:B:344:ALA:O	2:B:348:LEU:HB2	2.17	0.44
2:D:193:CYS:O	2:D:241:ARG:HD2	2.18	0.44
2:B:199:TYR:CE2	2:B:348:LEU:HD21	2.52	0.44
2:B:183:HIS:HB2	2:B:317:GLN:NE2	2.29	0.44
1:A:163:VAL:HA	6:A:440:HOH:O	2.18	0.44
1:C:227:TRP:HB3	1:C:230:VAL:CG2	2.48	0.44
1:C:221:THR:CG2	1:C:243:TRP:H	2.31	0.43
1:A:134:LEU:HD21	3:A:301:1RO:O1	2.17	0.43
2:D:399:LEU:HD23	2:D:426:PRO:HB2	2.00	0.43
2:B:328:LYS:HZ1	2:B:424:LEU:HD21	1.84	0.43
3:C:301:1RO:N2	3:C:301:1RO:C23	2.81	0.43
1:A:71:HIS:CD2	1:A:76:LEU:HD13	2.54	0.43
2:D:233:HIS:HD2	6:D:603:HOH:O	2.00	0.43
1:C:72:THR:OG1	1:C:73:GLU:C	2.61	0.43
1:A:295:HIS:HD2	1:A:297:ARG:CA	2.32	0.43
1:A:65:LYS:HB2	1:A:65:LYS:HE3	1.85	0.42
1:A:268:HIS:HD2	6:A:509:HOH:O	2.01	0.42
1:A:60:HIS:HE1	6:A:430:HOH:O	2.02	0.42
1:A:71:HIS:HA	1:A:72:THR:HA	1.86	0.42
2:B:233:HIS:HD2	6:B:602:HOH:O	2.02	0.42
1:A:1:MET:HE1	1:A:32:LEU:HD13	2.02	0.42
1:C:252:VAL:CG2	1:C:255:LEU:HD12	2.45	0.42
2:D:395:HIS:HE1	2:D:427:PRO:O	2.03	0.42
1:C:181:SER:HB3	6:C:451:HOH:O	2.19	0.41
2:B:176:PRO:O	2:B:179[B]:HIS:HD2	2.02	0.41
1:A:14[A]:THR:CG2	1:A:148:LEU:HD13	2.50	0.41
2:D:373:PRO:HD2	2:D:376:LEU:HD12	2.03	0.41
1:A:17:VAL:HG23	1:A:34:LYS:HB3	2.03	0.41
1:A:37:LEU:HD13	2:B:296:HIS:NE2	2.35	0.41
1:A:52:ILE:CD1	1:A:78:LEU:HD21	2.46	0.41
2:D:378:ARG:HD2	2:D:378:ARG:HA	1.94	0.41
2:B:388:LYS:HB3	2:B:389:PRO:HD3	2.01	0.41
1:A:62:ASN:ND2	1:A:110:GLN:HB3	2.36	0.41
1:C:222:PRO:HD3	1:C:269:TYR:CZ	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:VAL:HA	1:A:45:PRO:HD3	1.96	0.41
2:D:199:TYR:CD1	2:D:199:TYR:C	2.99	0.41
2:D:203:GLN:HA	2:D:204:PRO:HD3	1.92	0.40
1:C:71:HIS:HB3	1:C:72:THR:H	1.18	0.40
2:D:202:LYS:O	2:D:204:PRO:HD3	2.22	0.40
2:D:345:ASP:HA	2:D:346:PRO:HA	1.92	0.40
2:B:345:ASP:HA	2:B:346:PRO:HA	1.88	0.40
2:D:183:HIS:CD2	2:D:379:LYS:HE3	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	297/300 (99%)	285 (96%)	9 (3%)	3 (1%)	12	8
1	C	297/300 (99%)	287 (97%)	9 (3%)	1 (0%)	36	35
2	B	257/258 (100%)	255 (99%)	2 (1%)	0	100	100
2	D	253/258 (98%)	247 (98%)	6 (2%)	0	100	100
All	All	1104/1116 (99%)	1074 (97%)	26 (2%)	4 (0%)	30	27

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	162	GLU
1	A	164	VAL
1	C	164	VAL
1	A	163	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	265/263 (101%)	255 (96%)	10 (4%)	29	29
1	C	264/263 (100%)	252 (96%)	12 (4%)	24	23
2	B	233/232 (100%)	227 (97%)	6 (3%)	40	44
2	D	229/232 (99%)	219 (96%)	10 (4%)	25	24
All	All	991/990 (100%)	953 (96%)	38 (4%)	28	29

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	ILE
1	A	36	ARG
1	A	55	LEU
1	A	72	THR
1	A	96	LEU
1	A	148	LEU
1	A	150	ARG
1	A	161	HIS
1	A	162	GLU
1	A	163	VAL
2	B	196	LYS
2	B	232	LEU
2	B	281	ILE
2	B	285	THR
2	B	292	LEU
2	B	296	HIS
1	C	34	LYS
1	C	37	LEU
1	C	55	LEU
1	C	72	THR
1	C	73	GLU
1	C	101	LEU
1	C	103	LEU
1	C	150	ARG

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Mol	Chain	Res	Type
1	C	202	LEU
1	C	230	VAL
1	C	278	LYS
1	C	281	LEU
2	D	196	LYS
2	D	232	LEU
2	D	245	SER
2	D	250	ARG
2	D	292	LEU
2	D	296	HIS
2	D	328	LYS
2	D	348	LEU
2	D	384	LEU
2	D	428	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	HIS
1	A	74	ASN
1	A	265	GLN
1	A	295	HIS
2	B	228	GLN
2	B	233	HIS
2	B	254	GLN
2	B	395	HIS
2	B	403	GLN
2	B	425	ASN
1	C	60	HIS
1	C	62	ASN
1	C	74	ASN
1	C	85	GLN
1	C	119	HIS
1	C	161	HIS
1	C	246	GLN
1	C	265	GLN
2	D	233	HIS
2	D	254	GLN
2	D	313	GLN
2	D	317	GLN
2	D	395	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	TPO	C	160	1	8,10,11	0.91	0	10,14,16	0.95	0
1	TPO	A	160	1	8,10,11	0.91	0	10,14,16	1.20	1 (10%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	TPO	C	160	1	-	1/9/11/13	-
1	TPO	A	160	1	-	0/9/11/13	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	160	TPO	O3P-P-O2P	2.19	116.00	107.80

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	160	TPO	O-C-CA-CB

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	SGM	B	501	-	5,5,5	0.51	0	5,5,5	0.65	0
3	1RO	A	301	-	27,27,27	3.07	4 (14%)	37,37,37	3.71	15 (40%)
3	1RO	C	301	-	27,27,27	3.04	5 (18%)	37,37,37	3.51	14 (37%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SGM	B	501	-	-	1/4/4/4	-
3	1RO	A	301	-	-	3/9/21/21	0/4/4/4
3	1RO	C	301	-	-	3/9/21/21	0/4/4/4

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	301	1RO	C11-C12	13.90	1.49	1.34
3	C	301	1RO	C11-C12	13.84	1.49	1.34
3	A	301	1RO	C3-C4	4.34	1.48	1.42
3	C	301	1RO	C3-C4	4.31	1.48	1.42
3	A	301	1RO	C13-N2	-2.78	1.32	1.38
3	A	301	1RO	O1-C13	2.52	1.28	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	301	1RO	C13-N2	-2.45	1.32	1.38
3	C	301	1RO	O1-C13	2.42	1.28	1.23
3	C	301	1RO	C15-N2	2.11	1.34	1.31

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	301	1RO	N3-C15-N2	-11.49	114.96	123.99
3	A	301	1RO	C1-C11-C12	-11.22	115.83	130.92
3	C	301	1RO	N3-C15-N2	-10.54	115.71	123.99
3	C	301	1RO	C1-C11-C12	-10.33	117.03	130.92
3	C	301	1RO	C12-C13-N2	7.52	118.01	113.43
3	A	301	1RO	S1-C15-N3	7.47	129.12	121.32
3	A	301	1RO	C12-C13-N2	7.34	117.90	113.43
3	C	301	1RO	S1-C15-N3	6.74	128.36	121.32
3	C	301	1RO	C13-C12-S1	-5.94	105.64	109.15
3	A	301	1RO	C13-C12-S1	-5.64	105.82	109.15
3	C	301	1RO	C11-C12-C13	5.16	127.14	122.24
3	A	301	1RO	C11-C12-C13	5.14	127.12	122.24
3	A	301	1RO	O1-C13-C12	3.82	125.42	122.59
3	A	301	1RO	O1-C13-N2	-3.69	116.67	124.27
3	C	301	1RO	O1-C13-N2	-3.33	117.41	124.27
3	C	301	1RO	C9-N1-C4	2.75	121.10	116.93
3	C	301	1RO	C22-C21-S2	-2.70	106.41	113.02
3	A	301	1RO	C9-N1-C4	2.70	121.02	116.93
3	C	301	1RO	O1-C13-C12	2.68	124.57	122.59
3	A	301	1RO	C22-C21-S2	-2.65	106.54	113.02
3	C	301	1RO	C5-C4-N1	2.59	122.71	118.55
3	A	301	1RO	C5-C4-N1	2.47	122.52	118.55
3	A	301	1RO	C3-C4-N1	-2.41	118.72	122.03
3	C	301	1RO	C3-C4-N1	-2.39	118.74	122.03
3	A	301	1RO	C18-N3-C15	-2.31	118.53	122.14
3	A	301	1RO	C18-C19-C23	2.28	134.32	127.56
3	C	301	1RO	C18-C19-C23	2.22	134.16	127.56
3	C	301	1RO	C18-N3-C15	-2.18	118.72	122.14
3	A	301	1RO	C18-C19-S2	-2.05	117.64	121.44

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	301	1RO	C1-C11-C12-C13

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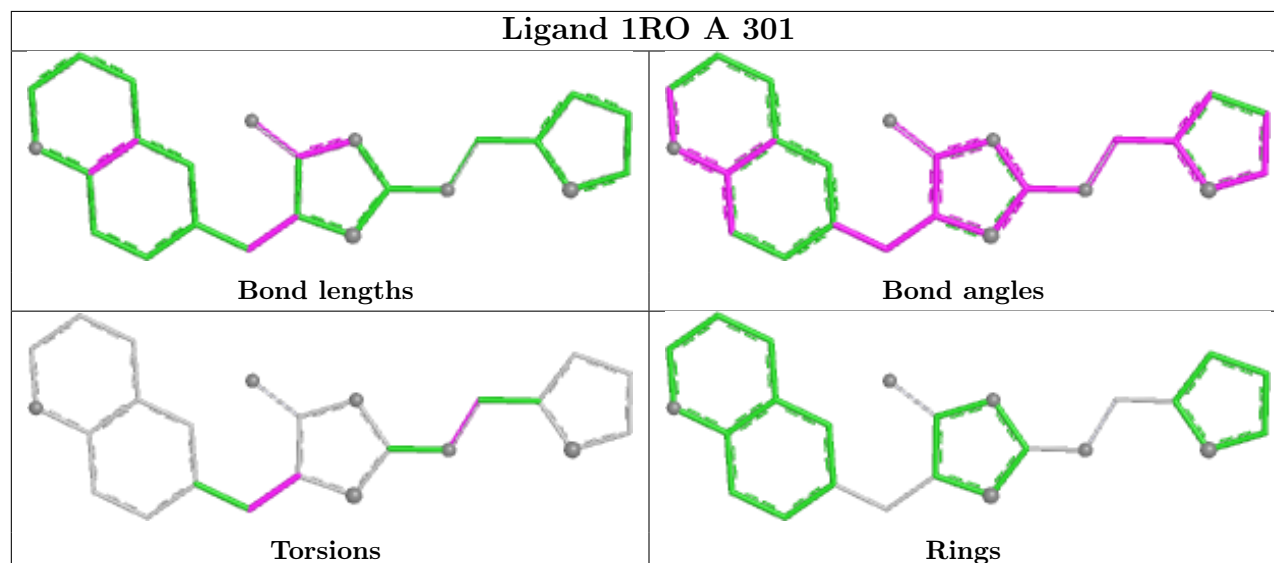
Mol	Chain	Res	Type	Atoms
3	C	301	1RO	C1-C11-C12-C13
4	B	501	SGM	S1-C1-C2-O2
3	A	301	1RO	C19-C18-N3-C15
3	C	301	1RO	C19-C18-N3-C15
3	A	301	1RO	C1-C11-C12-S1
3	C	301	1RO	C1-C11-C12-S1

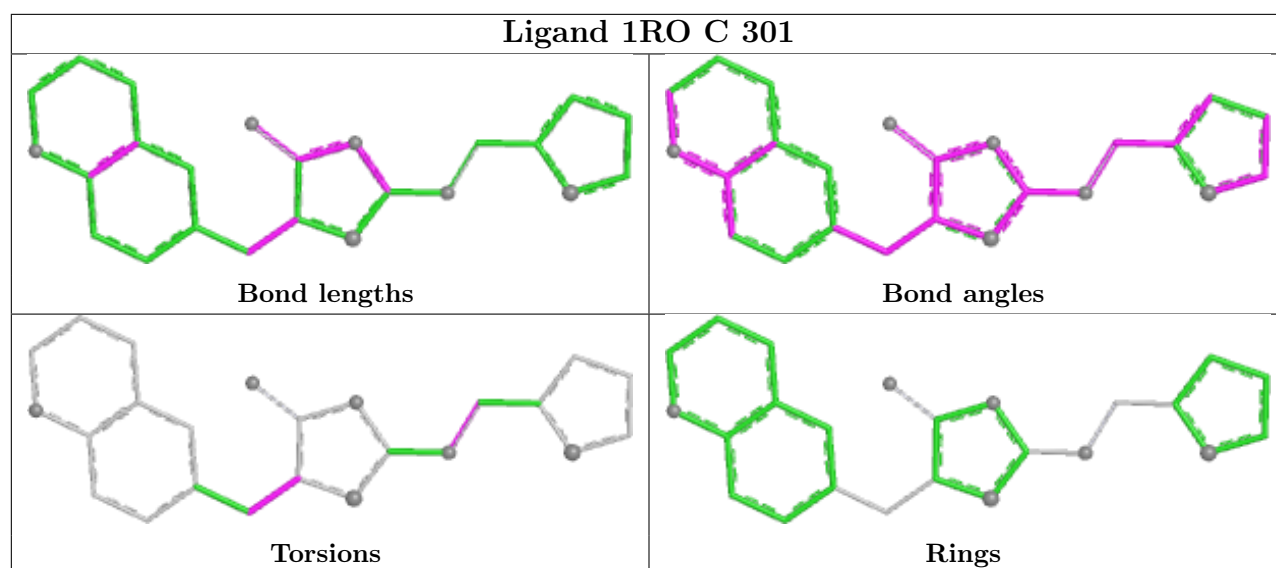
There are no ring outliers.

3 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	501	SGM	1	0
3	A	301	1RO	9	0
3	C	301	1RO	9	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	297/300 (99%)	0.25	17 (5%) 29 28	9, 24, 43, 86	4 (1%)
1	C	296/300 (98%)	0.73	30 (10%) 12 11	12, 33, 51, 76	3 (1%)
2	B	257/258 (99%)	0.70	29 (11%) 10 9	13, 34, 52, 76	2 (0%)
2	D	255/258 (98%)	0.92	46 (18%) 3 3	18, 34, 62, 87	0
All	All	1105/1116 (99%)	0.64	122 (11%) 10 9	9, 31, 55, 87	9 (0%)

All (122) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	175	VAL	9.8
2	D	176	PRO	9.2
1	A	72	THR	7.2
1	A	-2	PRO	7.1
2	D	429	THR	6.0
1	C	72	THR	5.9
2	D	428	GLU	5.5
1	A	71	HIS	5.3
1	C	295	HIS	5.2
2	D	177	ASP	5.1
1	A	39	THR	5.1
2	B	432	LEU	5.0
2	B	176	PRO	4.8
1	C	162	GLU	4.7
2	D	323	GLN	4.5
1	A	2	GLU	4.2
1	A	38	ASP	4.0
1	A	73	GLU	3.9
1	C	71	HIS	3.9
2	B	177	ASP	3.9
2	D	178	TYR	3.7

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Mol	Chain	Res	Type	RSRZ
2	D	378	ARG	3.7
1	C	296	LEU	3.6
1	C	74	ASN	3.5
1	A	178	LYS	3.4
1	C	161	HIS	3.3
2	D	386	SER	3.3
1	C	230	VAL	3.3
1	A	0	SER	3.3
2	D	374	GLU	3.2
2	B	207	THR	3.2
2	D	384	LEU	3.2
2	D	328	LYS	3.1
2	D	179	HIS	3.1
2	B	284	ASP	3.0
2	B	283	ASP	3.0
2	B	385	GLU	3.0
1	C	0	SER	2.9
2	D	367	VAL	2.9
2	B	280	TYR	2.9
2	D	284	ASP	2.9
1	A	-1	GLY	2.9
2	B	282	THR	2.9
2	D	322	GLN	2.9
2	B	378	ARG	2.9
1	C	221	THR	2.9
2	D	324	PRO	2.9
1	A	161	HIS	2.9
1	C	238	PRO	2.8
1	C	248	PHE	2.8
1	A	37	LEU	2.8
2	B	285	THR	2.8
1	C	73	GLU	2.7
1	C	97	THR	2.7
2	D	285	THR	2.7
1	C	120	SER	2.7
2	B	288	LYS	2.7
2	B	428	GLU	2.7
2	D	381	GLY	2.7
2	D	383	THR	2.7
2	D	373	PRO	2.7
2	B	430	LEU	2.6
2	D	377	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
2	D	365	TYR	2.6
2	D	372	TRP	2.6
1	C	252	VAL	2.6
1	C	198	THR	2.6
1	C	231	THR	2.6
2	B	431	ASN	2.6
2	D	418	TYR	2.6
1	C	35	ILE	2.6
2	D	327	CYS	2.5
2	D	198	GLY	2.5
2	D	371	SER	2.5
1	C	287	GLN	2.5
2	B	377	ILE	2.5
2	B	197	VAL	2.5
1	C	223[A]	ASP	2.4
1	C	225	VAL	2.4
1	C	226	VAL	2.4
2	B	296	HIS	2.4
2	D	423	LEU	2.4
2	D	416	SER	2.4
2	B	271	TYR	2.4
1	A	97	THR	2.4
2	B	198	GLY	2.4
2	D	364	LEU	2.3
2	D	362	LEU	2.3
2	D	419	HIS	2.3
2	D	392	MET	2.3
2	B	400	LYS	2.3
2	D	281	ILE	2.3
1	A	162	GLU	2.2
2	D	197	VAL	2.2
1	C	233	MET	2.2
2	D	282	THR	2.2
2	B	324	PRO	2.2
1	A	179	TYR	2.2
2	B	287	THR	2.2
2	B	323	GLN	2.2
1	C	258	ASP	2.2
1	A	10	ILE	2.2
2	D	326	ASN	2.2
1	C	101	LEU	2.1
2	D	414	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
2	D	359	ALA	2.1
1	C	213	PHE	2.1
2	B	403	GLN	2.1
1	C	273	LYS	2.1
2	D	280	TYR	2.1
2	B	371	SER	2.1
1	C	165[A]	THR	2.1
2	D	388	LYS	2.1
2	D	325	ALA	2.1
1	C	2	GLU	2.0
2	B	411	GLU	2.0
2	D	366	THR	2.0
1	A	268	HIS	2.0
2	D	320	LEU	2.0
2	D	387	LEU	2.0
2	B	289	LYS	2.0
2	B	179[A]	HIS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	TPO	A	160	11/12	0.98	0.06	20,21,22,23	0
1	TPO	C	160	11/12	0.98	0.06	23,25,28,28	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

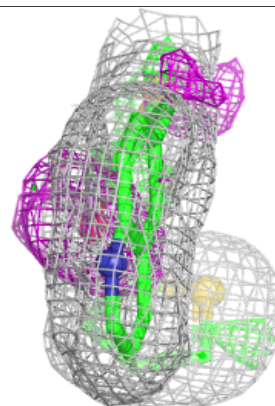
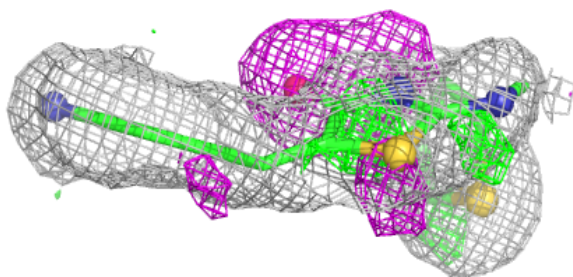
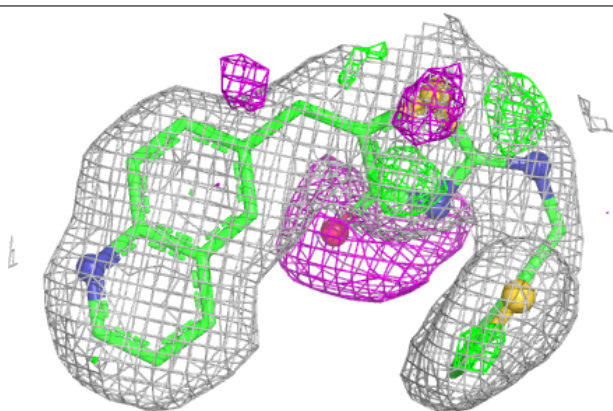
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

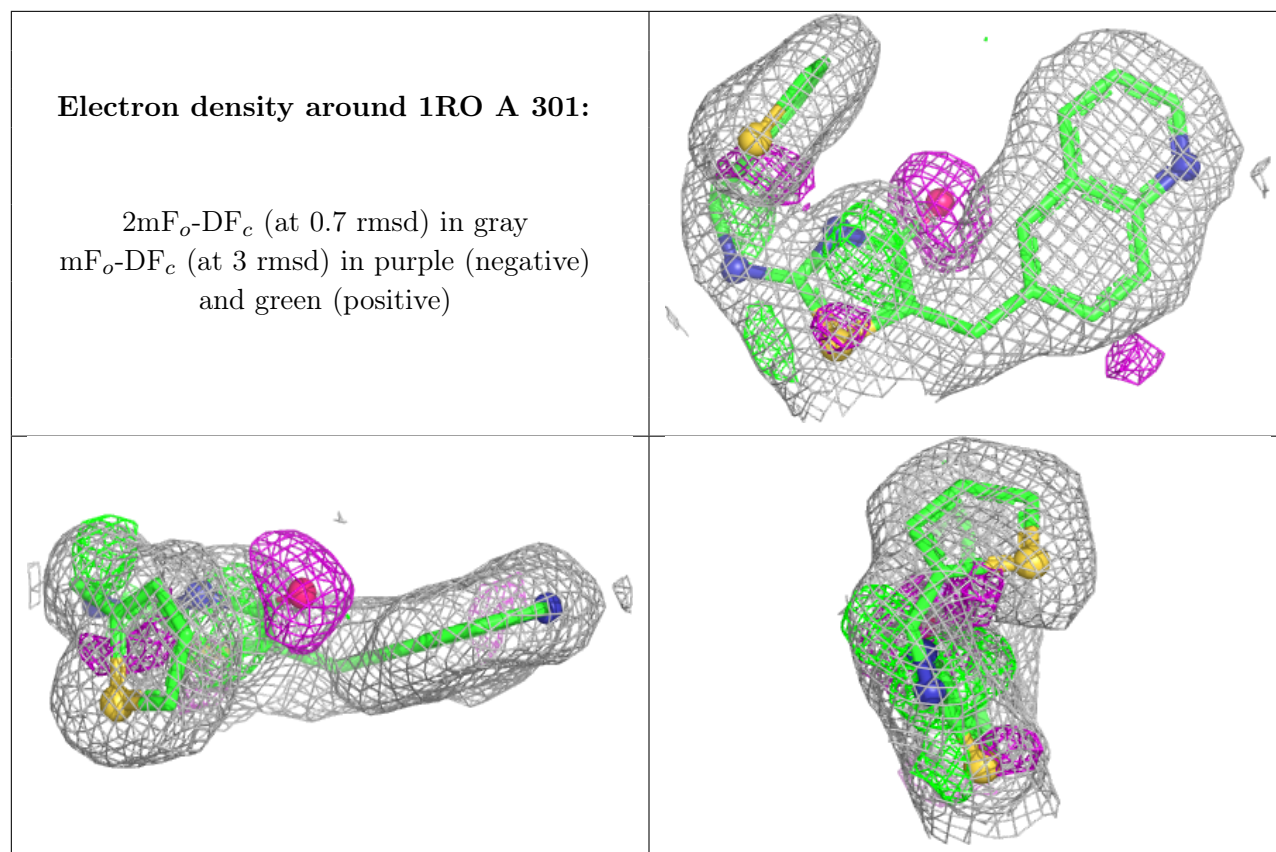
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	1RO	C	301	24/24	0.83	0.14	29,32,36,38	0
3	1RO	A	301	24/24	0.86	0.12	24,29,32,35	0
5	MG	D	501	1/1	0.89	0.17	29,29,29,29	0
4	SGM	B	501	6/6	0.90	0.17	41,42,46,54	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around 1RO C 301:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers [i](#)

There are no such residues in this entry.